HELIUM MEDIATED DEPOSITION ON THE TiO_2(110) SURFACE FROM FIRST-PRINCIPLES

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Helium droplets serve not only as a cryogetic matrix for high-resolution molecular spectroscopy [1]. This way, very recent experimental measurements [2] have shown that helium droplets can act as carriers for the “soft-landing” deposition of catalytic and photocatalytic species, formed inside the droplets, on the surface of different substrates. The development of these soft-landing techniques is very important in many areas such the controlled synthesis of nano-structured metal/TiO_2 photo-catalysts (e.g., to optimize the separation between photo-generated hole and electron carriers). A microscopic understanding of these processes requires, at a first step, first-principle simulations of the helium droplet collision dynamics at impact with the surface. These theoretical studies face, at least, two challenges: the proper description of long-range dynamical correlation (dispersion) effects in extended systems (e.g., by using embedded cluster modeling), and the application of a quantum-mechanical formalism to describe the helium-droplet dynamics. By choosing the TiO_2(110) surface as a technologically relevant substrate, we will show our latest progresses in this emerging area of helium droplet research [3].

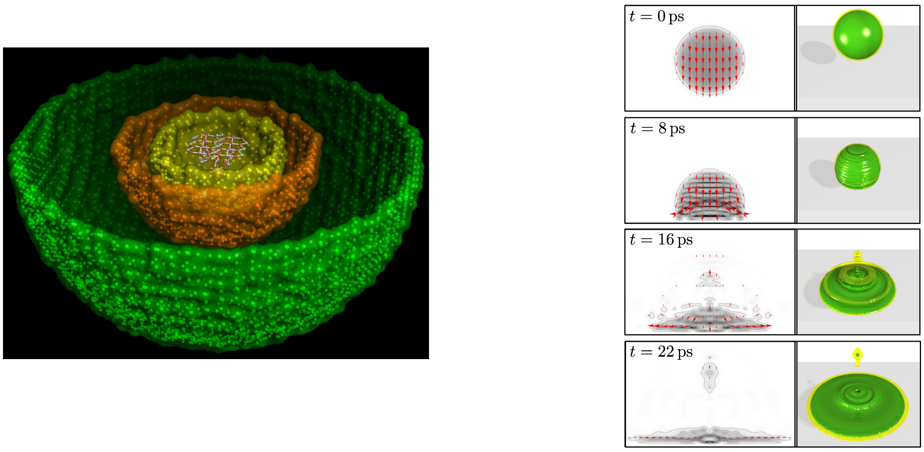

Figure: Left: Embedded cluster modeling of the He-TiO_2(110) extended system. Right: Quantum-dynamics of a helium droplet at impact with the TiO_2(110) surface from Ref. 3.

<u>References</u>

[1] C. Callegari and W. E. Ernst, Handbook of High-resolution Spectroscopy, Eds: M. Quack and F. Merkt. (2011) John Wiley & Sons.
[2] L. F. Gómez, E. Loginov, and A. F. Vilesov, Phys. Rev. Lett. 108, 155302 (2012).
[3] N. F. Aguirre, D. Mateo, A. O. Mitrushchenkov, M. Pí, M. P. de Lara-Castells, J. Chem. Phys. **136**, 124703 (2012), Virtual Journal of Nanoscale Science & Technology **25**, Issue 15 (2012).